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JOURNAL OF
 COMPUTATIONAL AND
 APPLIED MATHEMATICS

Journal of Computational and Applied Mathematics 154 (2003) 161–173

www.elsevier.com/locate/cam

Fourier–Legendre approximation of a probability density from discrete data

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Received 1 December 2001; received in revised form 16 September 2002

Abstract

We produce a positive approximation of a probability density in $[0, 1]$ when only a finite number of values (possibly affected by noise) is available. This approximation is obtained by computing a number of Legendre–Fourier coefficients and applying the Maximum Entropy method. An example of application of this procedure is data-smoothing in the numerical solution of an identification problem for Fokker–Planck equation.

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1. Introduction. Position of the problem

We suppose to collect N values of a positive probability density $u: [0, 1] \rightarrow \mathbb{R}$ in the N distinct points $x_1, \dots, x_N \in (0, 1)$. Experimental values can be modelled by the vector $\tilde{u} = (\tilde{u}_k)_{k=1}^N$ defined as

$$\tilde{u} = U(1 + \delta u), \quad (1.1)$$

where $U = (u(x_k))_{k=1}^N$ and $\delta u = (\delta u_k)_{k=1}^N$. Assume that $\sum_{k=1}^N (\delta u_k)^2 \leq \varepsilon^2$. Clearly, $u(x_k) > 0$ but we cannot say that $\tilde{u}_k \geq 0$.

Remark. It could be more appropriate to regard δu as a vector of N pairwise independent normal random variables with mean equal to zero and assigned variance. Nevertheless, actually this is not relevant at the present stage.

In what follows it is $\|\cdot\| \equiv \|\cdot\|_2$.

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In order to transform the N -dimensional vector \tilde{u} in a regular function $\tilde{u}^N: [0, 1] \rightarrow (0, \infty)$ we will carry on the following smoothing procedure:

1. Determine the first N (perturbed) Fourier–Legendre coefficients (FLC) of u from the data vector \tilde{u} ;
2. Compute the Maximum Entropy solution \tilde{u}^N of the corresponding generalized moment problem;

Then, we estimate stability and accuracy of the approximation produced.

Finally, in Section 3 we verify that $u^N \approx u$ is a suitable input data for numerical solution of an identification problem for Fokker–Planck equation.

2. The smoothing procedure

2.1. Step 1: Fourier–Legendre coefficients

The k th FLC of u is defined as $\lambda_k = \int_0^1 u(x) L_k(x) dx$ where L_k is the Legendre polynomial of degree k shifted in $[0, 1]$ with $L_k(1) = 1$. We want to compute $\lambda_0, \dots, \lambda_{N-1}$ from the knowledge of the N values $U_k = u(x_k^{(N)})$. Here, the numbers $x_k^{(N)}$ are the zeros of the $(N+1)$ th shifted Legendre polynomial L_N . We have $\sum_{i=1}^N L_{i-1}(x_j^{(N)}) \lambda_{i-1} = U_j$ for $j = 1, \dots, N$ i.e.,

$$(V^L)^T \lambda = U.$$

Here, V^L is a Vandermonde-like matrix whose element of position (i, j) is $v_{ij} = L_{i-1}(x_j^{(N)})$ (we recall that A^T means the matrix A transposed). It is known that this linear system is quite well conditioned. More precisely there is numerical evidence that the condition number (relative to the Frobenius norm) of V^L is approximately N [7]. In [7] is also proved the following rigorous result: the (Frobenius) condition number of V^L is $\kappa_N^L = \sqrt{\sum_{k=1}^N w_k \sum_{k=1}^N 1/w_k}$ where the w_k 's are the Christoffel weights corresponding to the abscissas $x_k^{(N)}$. Straightforward calculations based on [18, formula (15.3.10)] lead to the not optimal (but significant) estimate $\kappa_N^L \leq N^{3/2}$.

Suppose that U is affected by noise like in (1.1). In this case $\tilde{\lambda}$ is a vector of *perturbed* LFCs. We have

$$V^L \tilde{\lambda} = \tilde{u}$$

and, after the previous discussion about conditioning of Vandermonde-like matrices, we write the classical estimate

$$\frac{\|\delta \lambda\|}{\|\lambda\|} \leq N^2 \frac{\|\delta U\|}{\|U\|} \quad (2.1)$$

with $\delta \lambda = \tilde{\lambda} - \lambda$ (see, for example [8] Chapter 1). Alternative methods for obtaining λ are described in Section 4.

2.2. Step 2: Maximum Entropy method

Recall that we are carrying on a smoothing procedure involving a finite set of pointwise measurements. Since our goal is to approximate a continuous probability density u , we have chances

to apply Jaynes maximum entropy principle [13] in order to select one among the infinite densities having the same first N Fourier–Legendre coefficients $\lambda_0, \dots, \lambda_{N-1}$ ($\lambda_0 = 1$). The selected density is “... uniquely determined as the one which is maximally noncommittal with regard to missing information ...” [13].

In practice, we have to solve the following optimization problem:

Minimise the functional $\int_0^1 u(x) \ln u(x) dx$ in the set of the probability densities (i.e., $u \geq 0$ and $\int_0^1 u(x) dx = 1$) such that $\int_0^1 u(x) L_j(x) dx = \lambda_j$ for $j = 0, \dots, N-1$.

It is well known (see, for example [4]) that the minimiser takes the form

$$u^N(x) = \exp \left\{ \sum_{k=1}^N \alpha_k L_{k-1}(x) \right\},$$

where the coefficients α_k must be determined by solving the system of N nonlinear equations

$$\int_0^1 u^N(x) L_j(x) dx = \lambda_j \quad (2.2)$$

for $j = 0, \dots, N-1$.

Existence and uniqueness of the solution $\alpha \in \mathbb{R}^N$ of system (2.2), stated by physical intuition in [13], come from the rigorous analysis of [4, Theorem 3.3; 3]. The rigorous numerical approach to the computation of the Maximum Entropy solution of a finite moment problem [11] can be extended to the determination of u^N . Convergence in the information-theoretic distance $\|u - u^N\|_{IT} = \int_0^1 u(x) \ln u(x)/u^N(x) dx$ is proved in [3]. Uniform convergence is proved in [2].

2.3. Accuracy and stability

Here we deal with the conditioning of system (2.2). First of all we approximate the integral at the l.h.s. by means of a Gaussian quadrature formula and obtain

$$\sum_{i=1}^N L_{j-1}(x_i^{(N)}) \exp \left\{ \sum_{k=1}^N \alpha_k L_{k-1}(x_i^{(N)}) \right\} w_i^{(N)} + \omega_N^j = \lambda_{j-1} \quad (2.3)$$

for $j = 1, \dots, N$. The remainder ω_N^j is expected to decay very fast under suitable bounds on the derivatives of u (see, for example [8] Section 3.2.3 for its expression in terms of the N th derivative of the integrand).

We introduce the transformation $b(\alpha)$ where

$$b_i(\alpha_1, \dots, \alpha_N) = \exp \left\{ \sum_{k=1}^N \alpha_k L_{k-1}(x_i^{(N)}) \right\}$$

for $i = 1, \dots, N$.

If we neglect ω_N^j , Eq. (2.3) appears in vector form (from now on V means V^L) as

$$V^T \text{Diag}[w_i]_{i=1}^N b(\alpha) = V^{-1} U.$$

It is not difficult to check that $(V^T \text{Diag}[w]V)_{kj} = \int_0^1 L_k(x) L_j(x) dx$ so that $V^{-1} = V^T \text{Diag}[w]$. Hence, we have

$$b(\alpha) = U.$$

A reliable definition of the condition number of a nonlinear system of equations can be found in [16]: Given the equation

$$b(\alpha) = c, \quad (2.4)$$

where α and c are real N -dimensional vectors and $b: \mathbb{R}^N \rightarrow \mathbb{R}^N$ is C^∞ , the (relative asymptotic) condition number κ_N for solving (2.4) at c^0 is

$$\kappa_N = \frac{\|c^0\|}{\|\alpha^0\|} \| [Jb(\alpha^0)]^{-1} \|,$$

where α^0 is the solution of $b(\alpha) = c^0$ and Jb denotes the Jacobian matrix of b .

Remark. Reliability of Rice's definition of conditioning for non linear systems depends on the vectors c^0 and α^0 . If these vectors have elements of greatly varying orders of magnitude the condition number as defined can be grossly misleading [Gautschi, private communication]. In our case we are dealing with vectors made up by samples of u and FLC of $\log u$. This kind of vectors can be assumed enough gently behaving without great loss of generality.

It is easy to check that the Jacobian matrix of the transformation b at hand is

$$Jb(\alpha) = \text{Diag} \left[\exp \left\{ \sum_{k=1}^N \alpha_k L_{k-1}(x_i^{(N)}) \right\} \right]_{i=1}^N V^T$$

so that

$$\| [Jb(\alpha)]^{-1} \| \leq N^{3/2} \max_i \exp \left\{ - \sum_{k=1}^N \alpha_k L_{k-1}(x_i^{(N)}) \right\}. \quad (2.5)$$

To estimate the r.h.s. of (2.5) we make use of a known theorem about the convergence of maximum entropy solutions of finite moment problems:

Theorem BL (Borwein and Lewis [2]). *Let $u \in C^3(0,1)$ be a probability density continuous and strictly positive in $[0,1]$. Let $\lambda \in \mathbb{R}^N$ be the vector of its first N moments $\mu_k = \int_0^1 x^k u(x) dx$ ($k = 0, \dots, N-1$). Let u_N be the Maximum Entropy solution of the corresponding finite moment problem. We have*

$$\lim_{N \rightarrow \infty} u^N = u$$

uniformly in $[0,1]$. Moreover

$$\|u^N - u\|^2 \leq \frac{|(\log u)''|}{n^2}.$$

It is clear that if FLCs are available instead of moments, the maximum entropy approximant does not change.

Observe that, after Theorem BL, there exists a \bar{N} such that for any $N > \bar{N}$ we have

$$\min_{[0,1]} \exp \left\{ \sum_{k=1}^N \alpha_k L_{k-1}(x) \right\} \geq \frac{1}{2} \min_{[0,1]} u(x)$$

so that

$$\| [Jb(\alpha^0)]^{-1} \| \leq \frac{2N^{3/2}}{\min u} \quad (2.6)$$

for $N \geq \tilde{N}$.

Remark. In [4, Theorem 3.3] it is proved that if λ is the vector of the first FLCs of some probability density function (PDF), then Maximum Entropy approximant u^N exists and it is unique. If we start from perturbed data \tilde{u} and consequently produce perturbed FLCs $\tilde{\lambda}$, we are not sure that the maximum entropy approximant \tilde{u}^N exists. In fact, the set $F_N = \{(\lambda_1, \dots, \lambda_{N-1}) \in \mathbb{R}^{N-1} \text{ FLCs of a PDF}\}$ is open, bounded and convex [3] so that we have existence of \tilde{u}^N if ε is small enough. In particular, F^N is the convex hull of the curve $(L_1(t), \dots, L_{N-1}(t))_{t \in [0,1]}$. Moreover, observe that the role of F_N is the same of moment space D^N (see [14]) in finite Hausdorff moment problem. The geometry of D^N has been deeply studied, but very little seems to be known about F_N . So, it is proved that a ball included in D^N (convex hull of the curve $(t, \dots, t^{N-1})_{t \in [0,1]}$) must have diameter lower than $2^{-2(N-2)}$ ([14, Theorem 25.5]), but we can only conjecture that F^N is much less thin (probably “polynomially” thin) as a consequence of the orthogonality of Legendre polynomials.

At this point we can summarize our analysis in the following accuracy-stability estimate:

Theorem 2.1. Assume that u satisfies the hypothesis of Theorem BL and that $\min_{[0,1]} u(x) = \gamma > 0$. Recall that $\tilde{u} = U + \delta u$ and $(\sum_{k=1}^N (\delta u_k)^2 \leq \varepsilon^2)$. Let $u_N [\tilde{u}_N]$ be the Maximum Entropy solution of the generalized moment problem given the FLCs $\lambda [\tilde{\lambda}]$ derived from $U [\tilde{u}]$ if ε is small enough (see Remark). In our hypothesis, a positive integer \tilde{N} exists such that $\min_{[0,1]} u^N \geq \frac{\gamma}{2}$, $(\|u^N\|/\|u\|) \leq 2$ and $\|u^N - u\| \leq \frac{1}{2}$ when $N \geq \tilde{N}$. Hence, the following estimate holds when $N \geq \tilde{N}$:

$$\frac{\|\tilde{u}^N - u\|}{\|u\|} \leq \frac{1}{\gamma} \left\{ \frac{C}{N} + 2N^{3/2}\varepsilon \right\}. \quad (2.7)$$

Proof. We have

$$\|\tilde{u}^N - u\| \leq \|\tilde{u}^N - u^N\| + \|u - u^N\|.$$

Hence,

$$\begin{aligned} \frac{\|\tilde{u}^N - u^N\|}{\|u\|} &\leq \frac{\|u^N\|}{\|u\|} \|\tilde{u}^N - 1\| \\ &\leq \|\tilde{\alpha} - \alpha\|. \end{aligned}$$

At this point we abuse the concept of (relative asymptotic) condition number linearizing in some sense our problem. We have (in the notation of (2.4)):

$$\begin{aligned} \|\alpha - \tilde{\alpha}\| &\leq \|\alpha\| \kappa_N \frac{\|\delta U\|}{\|U\|} \\ &\leq \|[Jb(\alpha)]^{-1}\| \|\delta U\| \\ &\leq \frac{2N^{3/2}}{\gamma} \varepsilon. \end{aligned}$$

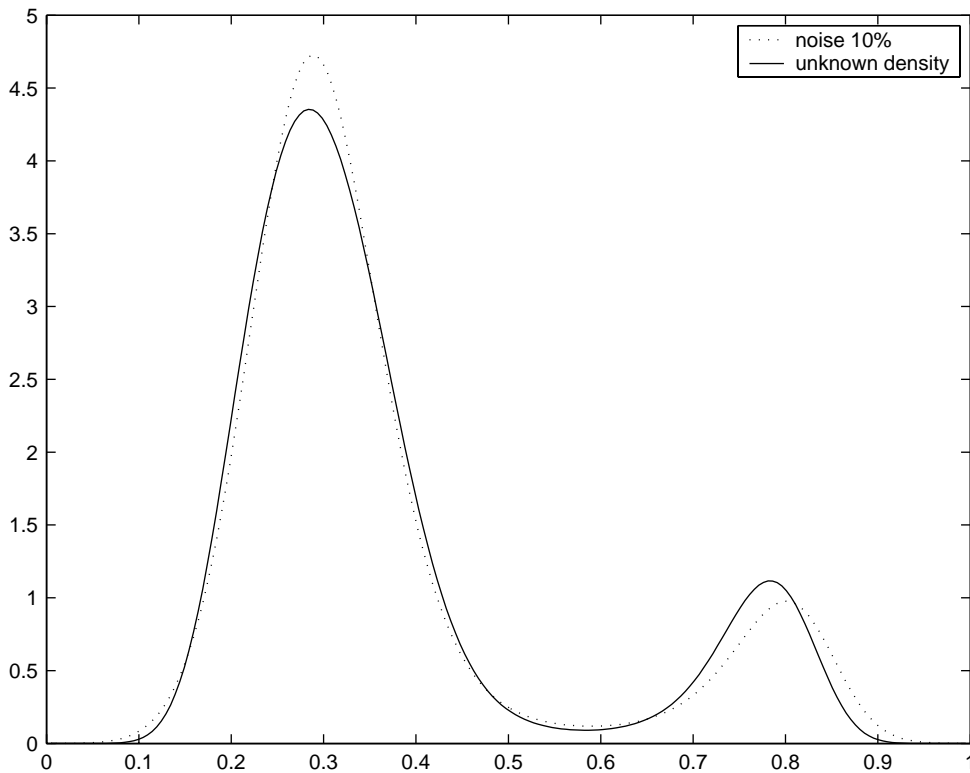


Fig. 1. Reconstruction from nine noisy Fourier-Legendre coefficients.

Finally, from (2.1) we obtain

$$\frac{\|\tilde{u}^N - u^N\|}{\|u\|} \leq \frac{2N^{3/2}}{\gamma} \varepsilon.$$

As for the discretization error we have

$$\|u - u^N\| \leq \frac{\sqrt{|(\log u)'''|}}{2N}$$

so that (2.7) is proved. \square

2.4. A numerical example

Results of previous subsection can be visualized by means of a numerical experiment whose output is reported in Fig. 1. Consider the probability density $u(x) = 5.86088 \dots \exp\{-0.027777 \dots (6x - 3)^6 - 4.16666 \dots \exp\{-36x^2 + 42x - 12.25\}\}$ in $[0, 1]$. Let $u^{(9)}$ be the maximum entropy approximant of Section 2.2 coming from exact values of the FL coefficients $\lambda_0, \dots, \lambda_8$. The approximation error is $(\|u - u^{(9)}\|/\|u\|) \approx 0.0463$. Let $u_\varepsilon^{(9)}$ come from the perturbed FL coefficients $\tilde{\lambda}_k = \lambda_k(1 + \varepsilon r_k)$ where $k = 0, \dots, 8$, $\varepsilon > 0$ and r_k is a random value in $(-1, 1)$. We observed that the error due to

magnification of noise (REM_N) becomes comparable with the approximation error only for $\varepsilon \approx 0.1$ (see the following table):

$$\begin{aligned}\varepsilon = 0.01 &\rightarrow \text{REM}_N = 0.0031 \\ \varepsilon = 0.05 &\rightarrow \text{REM}_N = 0.0047 \\ \varepsilon = 0.10 &\rightarrow \text{REM}_N = 0.0486 \\ \varepsilon = 0.50 &\rightarrow \text{REM}_N = 0.2547\end{aligned}$$

Remarks. It is interesting to compare (2.7) with analogous estimates regarding the classical finite moment problem. If we approximate a smooth function u by means of the polynomial \tilde{u}_N^P of best L^2 approximation, calculated from the first N noisy moments $\tilde{\mu}_k = \int_0^1 x^k u(x) dx + \delta u_k$ ($k = 0, \dots, N-1$) we get (see, for example [19])

$$\|\tilde{u}_N^P - u\| \leq \frac{\|u'\|}{2N} + \exp\{1.72 \dots N\} \varepsilon. \quad (2.8)$$

The same polynomial \tilde{u}_N^P could be obtained from noisy FLCs (see, for example [1]) showing essentially the same stability of (2.7). The maximum entropy solution u^N is anyway preferable in our context because of its positivity. Cancellation of typical Gibbs effect is also observed as an example of regularization after positivity assumption (see for example [6]).

3. An identification problem for elliptic PDE

Consider the problem of recovering a function V from observations about the evolution in time of the dynamical system

$$\dot{x} = -\frac{dV}{dx}. \quad (3.1)$$

Assume that the system is dissipative in the sense that a portion of the intrinsic information of the system itself gets lost along the evolution. It is clear that we have chances to identify attractors, but V (or its derivative f , the so-called drift) is underdetermined.

On the other hand, if we add a Langevin force to (3.1), we obtain the stochastic ODE (see [15,17])

$$dX_t = -\frac{dV}{dx}(X_t) dt + \sigma dW_t, \quad (3.2)$$

where $\sigma > 0$ is the *noise strength* of the Langevin perturbation (or diffusion coefficient). A solution of (3.2) (given the initial data $X_0 = x_0$ with probability one) is a Markov stochastic process. We have existence and uniqueness of X_t under suitable hypotheses that make no possible the explosion of the solution:

Theorem H (Has'minskiĭ [10, Theorem 3.4.1]). *Let $K \in \mathbb{R}$ a global attractor for (3.1). Assume that there is a bounded, open interval $(a, b) \in \mathbb{R}$ such that $K \subset (a, b)$ and there is a positive real number β such that $(dV/dx)(x)x \leq -\beta < 0$ for all $x \in \mathbb{R} \setminus (a, b)$. Then there exists a unique Markov process that solves the Cauchy problem (3.2) with initial data $X_0 = x_0$ (with probability 1).*

The transition probability densities $p(x, t|x_0, 0)$ are well known to solve the Fokker–Planck (FP) diffusion equation

$$\frac{\partial p}{\partial t}(x, t) = -\frac{d(fp)}{dx} + \frac{\sigma^2}{2} \frac{d^2 p}{dx^2} \quad (3.3)$$

with initial condition $p(x, 0) = \delta(x - x_0)$. Moreover, [10, Theorem 4.7.1] under suitable additional assumptions we have that $\forall x_0 \in \mathbb{R} \lim_{t \rightarrow \infty} p(x, t|x_0, 0) = u(x)$ in the sense of probability measures (densities p and u are Radon–Nykodim derivatives) where $u(x) = e^{-(2/\sigma^2)(V(x)-V(0))}$ is the unique solution of the stationary FP equation

$$-\frac{d(fp)}{dx} + \frac{\sigma^2}{2} \frac{d^2 p}{dx^2} = 0. \quad (3.4)$$

Now we are ready to state the following problem:

Given σ and u

Determine $V = \int f \, dx$.

It is easy to check that

$$V(x) = -\frac{\sigma^2}{2} \ln u(x).$$

If one is interested in the drift coefficient, it is $f(x) = -dV/dx = -u'/u \approx P'_N(x)$.

Observe that the inverse problem has been formulated in \mathbb{R} while the smoothing procedure in previous section regarded a density in $[0, 1]$. Since u is assumed analytical, we could continue it from $[0, 1]$ to \mathbb{R} . Moreover, we assumed that the system has a bounded global attractor K . Variable x could be rescaled so that $K \subset (0, 1)$. In practice, it is preferable that the interesting dynamics is observed mainly in $[0, 1]$.

Theorem BL in Section 2.2 suggests to construct a convergent sequence of stable approximations of the potential $V = -df/dx$. Hence, in the light of Section 1 we have

Theorem 3.1. *Let V be analytical in Ω_d (see Theorem BL in Section 2.3) and fulfill hypothesis of theorem H. Then, we have*

$$V(x) = -\lim_{N \rightarrow \infty} P_N(x)$$

and

$$f(x) = \lim_{N \rightarrow \infty} P'_N(x),$$

where $P_N(x) = \sum_{k=1, N} \alpha_k L_{k-1}(x)$. the numbers $\alpha_1, \dots, \alpha_N$ are obtained from the sample (1.1) using the method described in Sections 2.2 and 2.3. Limits are uniform in $[0, 1]$.

4. Variations on Step 1

4.1. Ergodicity

An alternative method for the determination of a finite number of FLCs of u can be formulated when the solution X_t of (3.2) is an *ergodic* Markov process for any initial condition.

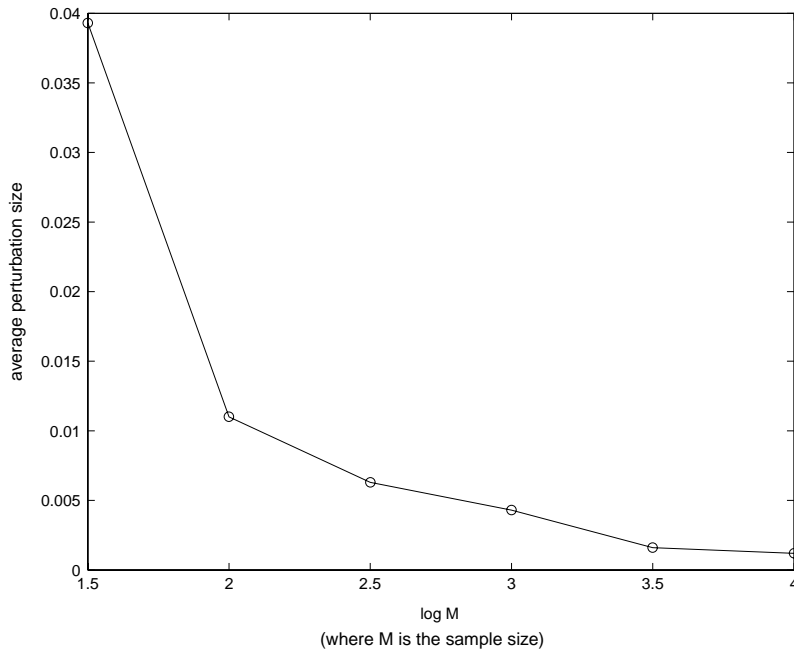


Fig. 2. Montecarlo method for computing FLCs from noisy samples (noise = 10%).

We recall that X_t is said to be ergodic if the following time average limit exists for a function ϕ and equals (w.p. 1) the spacial average with respect to the measure induced by u i.e.,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \phi(X_t) dt = \int_{\mathbb{R}} \phi(x) u(x) dx \quad (4.1)$$

for all measurable functions $\phi : \mathbb{R} \rightarrow \mathbb{R}$. Since (4.1) is usually quite difficult to verify directly, we assume that the following ergodicity criterion is verified [10, Section 4.4]:

There exists a bounded interval U such that if $x \in \mathbb{R} \setminus U$ the mean time $E_x \tau$ at which a path issuing from x reaches the set U is finite and $\sup_{x \in K} E_x \tau < \infty$ for all compact set $K \subset \mathbb{R}$.

We introduce the average FLC at time T

$$\lambda_k^T = \frac{1}{T} \int_0^T L_k(X_t) dt$$

so that

$$P \left\{ \lim_{T \rightarrow \infty} \lambda_k^T = \lambda_k \right\} = 1.$$

It means that w.p. 1 we have that $\forall \varepsilon > 0$ and N there is a T_N such that

$$\sqrt{\sum_{k=0}^N (\lambda_k^{T_N} - \lambda_k)^2} < \varepsilon.$$

Finally, the approximated random FLC $\lambda_k^{T_N}$ ($k = 0, \dots, N-1$) can be used as noisy data in step 2 of Section 1.

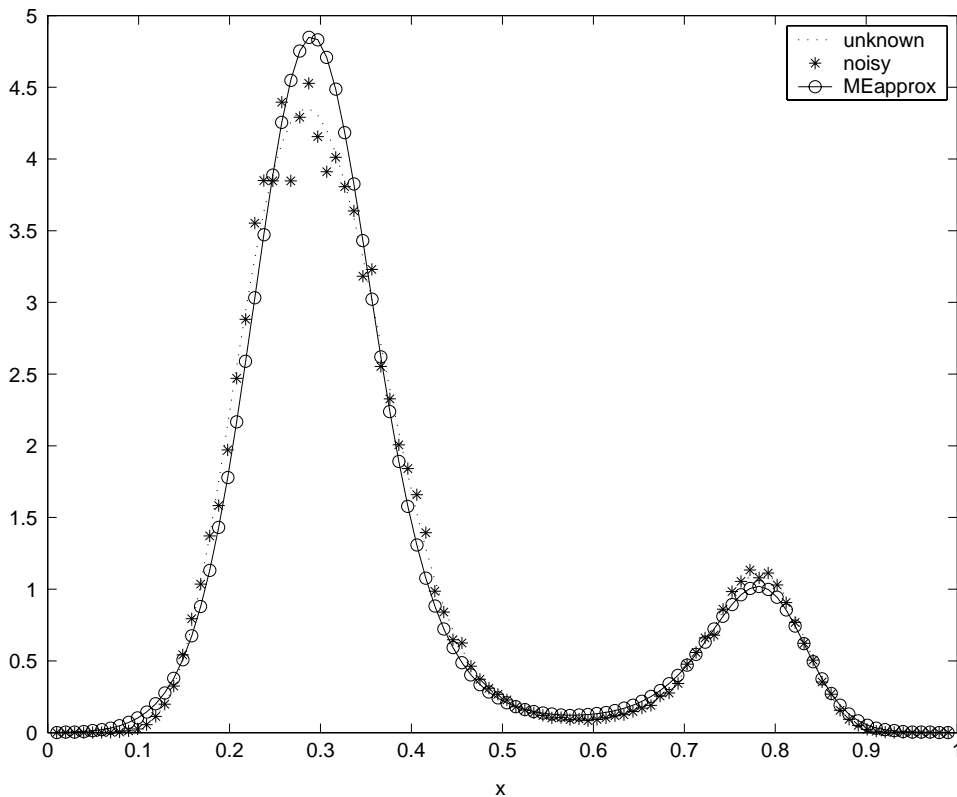


Fig. 3. Maximum entropy approximation of u from a noisy sample (100 points with noise = 10%) via Monte Carlo computation of its first eight FLCs.

4.2. Montecarlo

There is at least another interesting way to manage the vector $\tilde{u}_k = U_k + \delta u_k$ ($k = 1, \dots, M$) introduced in Section 1 to model the collection of data. We can obtain a number of approximated FLCs of u by way of a Montecarlo-like method without involving interpolation and with chances of reducing arbitrarily the size of the noise affecting the FLCs used for the construction of u^N . The method is based on the following Lemma that generalises a result in [12].

Lemma. Assume $\phi \in C^0[0, 1] : \forall \beta > 0$ and $\gamma > 0$ we have

$$P \left\{ \left| \int_0^1 \phi(x) \sum_{k=1}^M \delta u_k \delta(x - x_k^M) dx \right| < \beta \right\} > 1 - \gamma$$

for $M \geq \frac{\varepsilon^2}{\gamma \beta^2} \|\phi\|_2$.

Proof. It is sufficient to apply the classical Chebishev inequality (see for example [9, Section 32]). \square

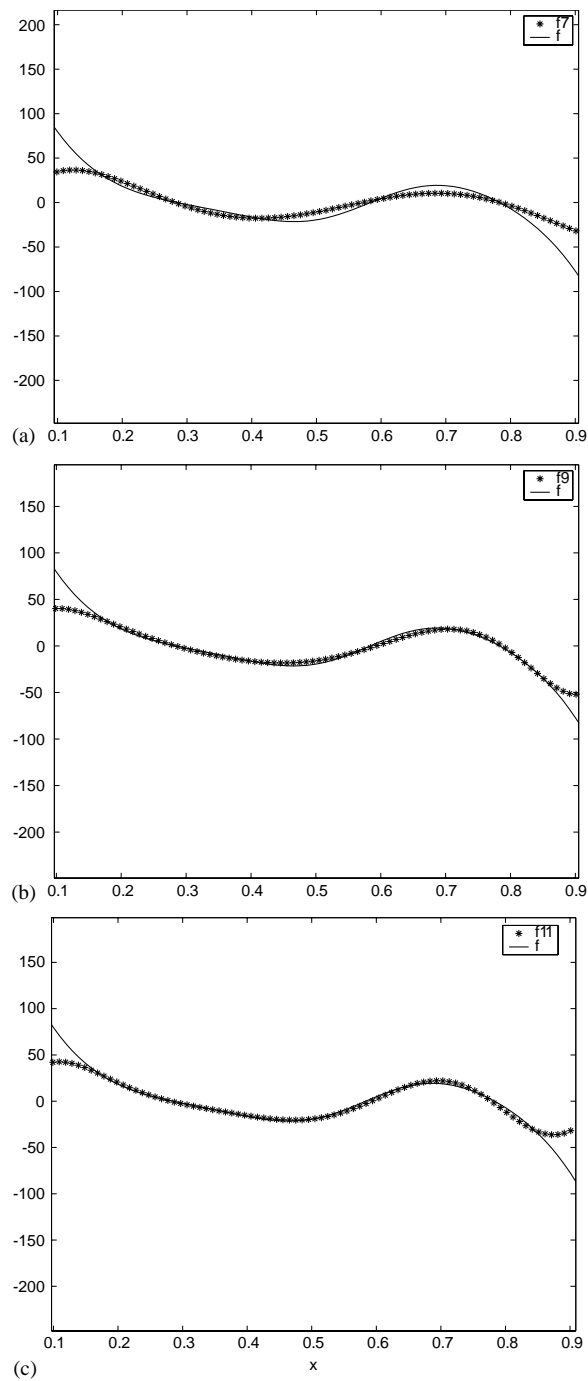


Fig. 4. Reconstruction of a nonlinear drift from data obtained by means of Montecarlo computations.

Since $\forall k = 1, 2, \dots$ it is $\|L_k\|_2 = 1$, we have

Corollary. *Let u satisfy the hypothesis of Theorem BL and let $\lambda_0, \dots, \lambda_{N-1}$ be the first FLCs of u . Then, $\forall \beta > 0$ and $\gamma > 0$ we have*

$$P \left\{ \left| \sum_{k=1}^M (U_k + \delta u_k) L_j(x_k^M) - \lambda_j \right| < \beta \right\} > 1 - \gamma$$

for $M \geq \max\{(4\varepsilon^2/\gamma\beta^2), \bar{M}\}$. Here, \bar{M} is such that $|\sum_{k=1}^{\bar{M}} (U_k + \delta u_k) L_j(x_k^{\bar{M}}) - \int_0^1 (U_k + \delta u_k) \delta(x - x_k^{\bar{M}}) L_j(x) dx| < \beta/2$.

We can conclude that the effect of a small perturbation of u on the computation of its FLCs goes to zero (with high probability) if $M \rightarrow \infty$.

In Fig. 2 we show results obtained in numerical experiments with the density u introduced in Section 2.4.

In Fig. 3 we can observe how much is nonsmooth the perturbed sample \tilde{u} . Nevertheless, the ME approximation from data obtained by means of Montecarlo computation actually looks not affected by noise. Finally, in Fig. 4 we show reconstructions of the drift $f = -(6x - 3)^5 + 50(6x - 3.5)e^{-(6x-3.5)^2}$ from \tilde{u} . It is possible to observe the expected uniform convergence in a subset of $[0, 1]$ that do not include zones in which u is very close to zero.

Remark. Since M will be usually very large, we will have in applications $N \ll M$. This fact suggests to consider the extension of properties of rectangular Vandermonde matrices [5] to rectangular Vandermonde-like matrices [Fasino-Inglese, work in progress].

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